



**IMT Nord Europe**  
École Mines-Télécom  
IMT-Université de Lille

# Graph Convolutional Networks (GCNs)

## Introduction to GCNs

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01.12.2023

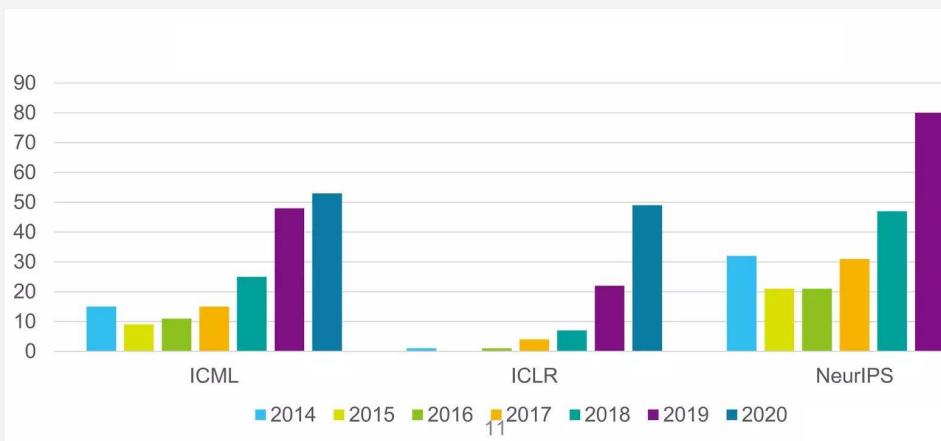


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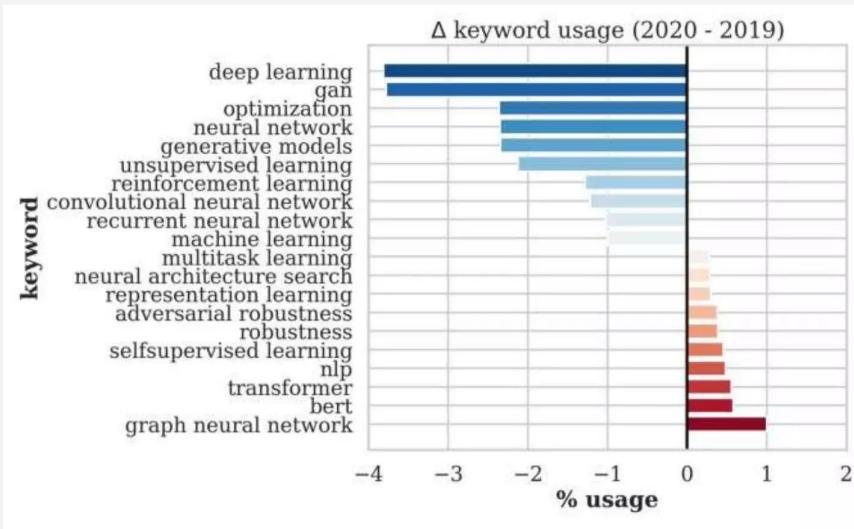
1. Why graphs ?
2. Fundamentals of graph structures.
  - a. Basic concepts
  - b. Graph data representation
  - c. Frameworks & utils
3. From CNNs to GCNs
  - a. Convolution on images
  - b. Convolution on graphs
4. GCNs
  - a. Tasks on graphs
  - b. Training GCNs
  - c. Practical advices
5. Take home notes
6. Practical example

## First, a few statistics

Number of accepted papers  
Title: "Graph"



ICLR submissions

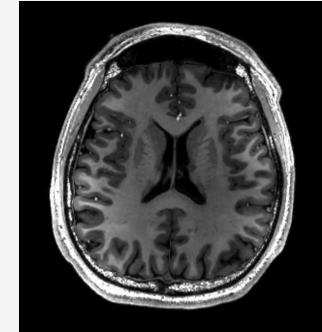


- ICML: International Conference on Machine Learning (rank A)
- ICLR: International Conference on Learning Representations (rank A\*)
- NeurIPS: Neural Information Processing Systems (rank A\*)

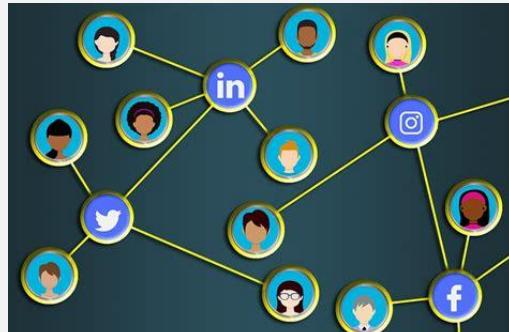
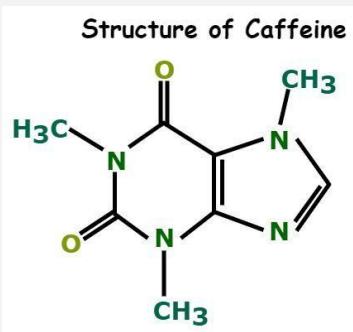
# 1. Why graphs ?

# Understanding Connectivity: Explore data beyond tabular and image formats

Image & sequential data...



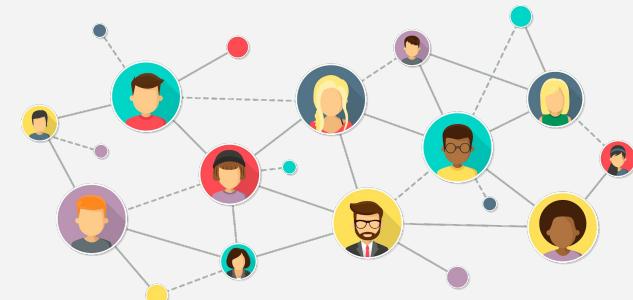
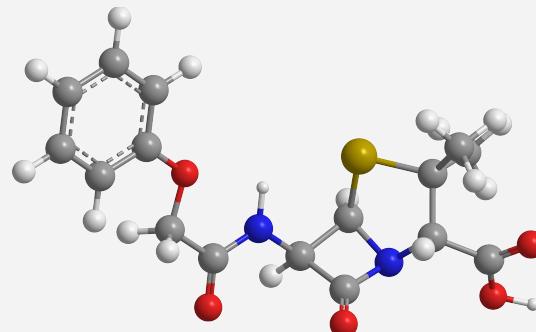
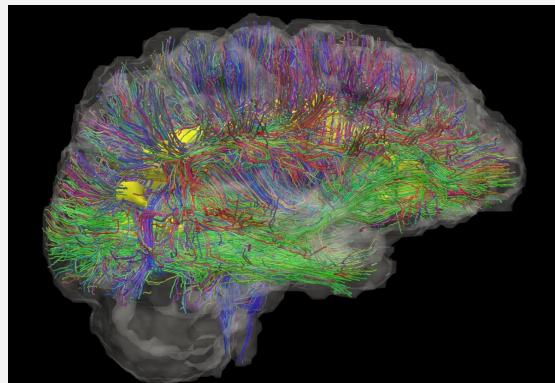
Graph structure data...



# Graphs are everywhere !

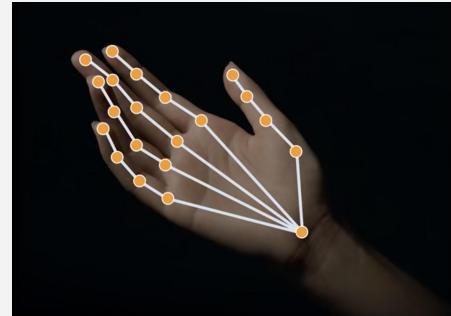
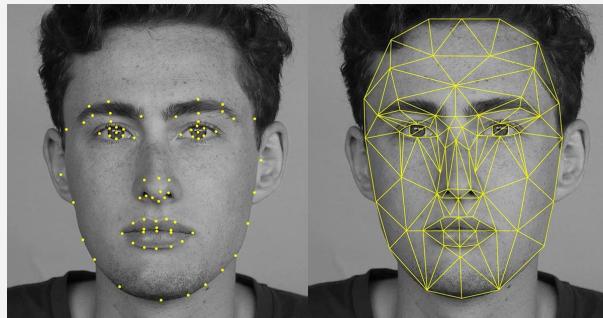
## *Why Graphs?*

Many problems are graphs in true nature. In our world, we see many data are graphs, such as molecules, social networks, and paper citations networks.



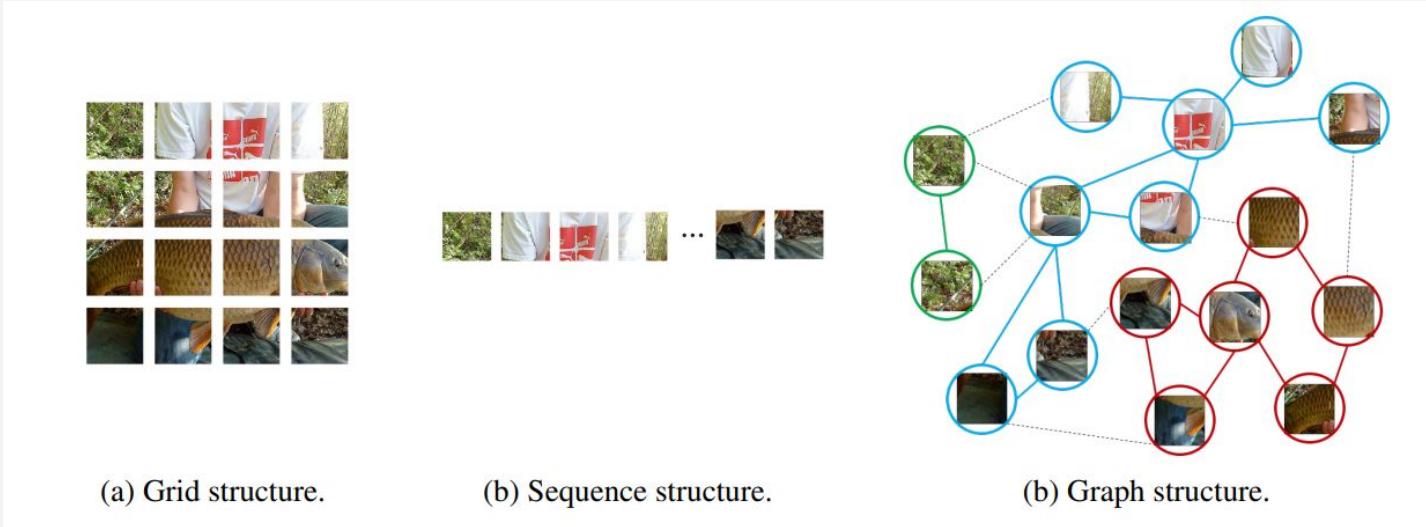
# Graphs are everywhere !

Even humans can be seen as graphs !



# Graphs are everywhere !

Even more surprising! Any image can be considered a graph!



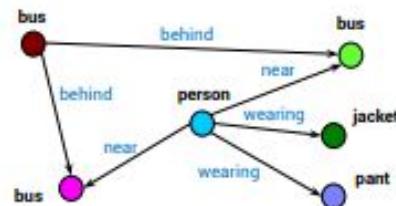
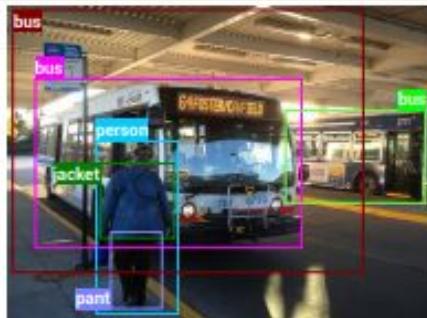
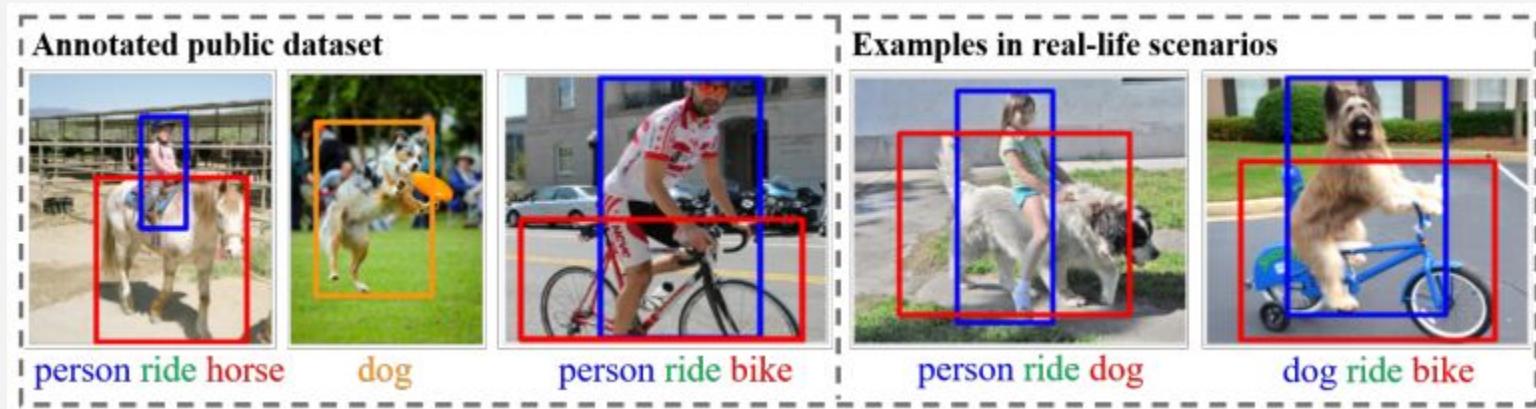
(a) Grid structure.

(b) Sequence structure.

(b) Graph structure.

# Graphs are everywhere !

Graphs are very useful in scene understanding



In a scene graph of an image:

- Nodes: objects
- Edges: relation between objects

## 2. Fundamentals of Graph Structure

# Graphs: Back to basics

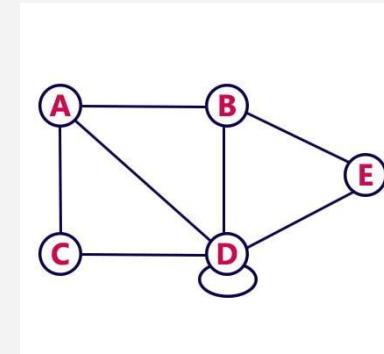
## What is a graph ?

A graph  $G=(V, E)$  is a set of points, called **nodes** or **vertices** ( $V$ ), which are interconnected by a set of lines called **edges** ( $E$ ).

$$V = \{v_1, v_2, v_3, \dots, v_n\}$$

$$E = \{(v_i, v_j), \dots\}$$

- Directed / Undirected
- Weighted / Unweighted



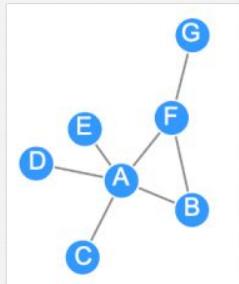
## What is an adjacency matrix ?

The adjacency matrix, also called the connection matrix, is a matrix containing rows and columns which is used to represent a graph connections, with 0 or 1 in the position of  $(v_i, v_j)$  according to the condition whether  $v_i$  and  $v_j$  are adjacent or not.

	A	B	C	D	E
A	0	1	1	1	0
B	1	0	0	1	1
C	1	0	0	1	0
D	1	1	1	1	1
E	0	1	0	1	0

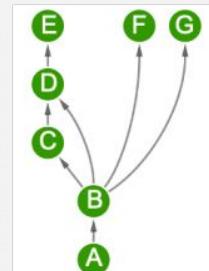
# Graphs: Back to basics

Undirected (unweighted)



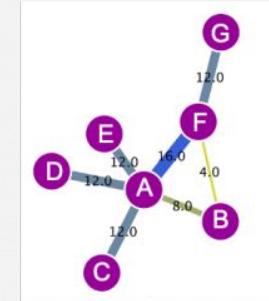
	A	B	C	D	E	F	G
A	0	1	1	1	1	1	0
B	1	0	0	0	0	1	0
C	1	0	0	0	0	0	0
D	1	0	0	0	0	0	0
E	1	0	0	0	0	0	0
F	1	1	0	0	0	0	1
G	0	0	0	0	0	1	0

Directed (unweighted)



	A	B	C	D	E	F	G
A	0	1	0	0	0	0	0
B	0	0	1	1	0	1	1
C	0	0	0	1	0	0	0
D	0	0	0	0	1	0	0
E	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0
G	0	0	0	0	0	0	0

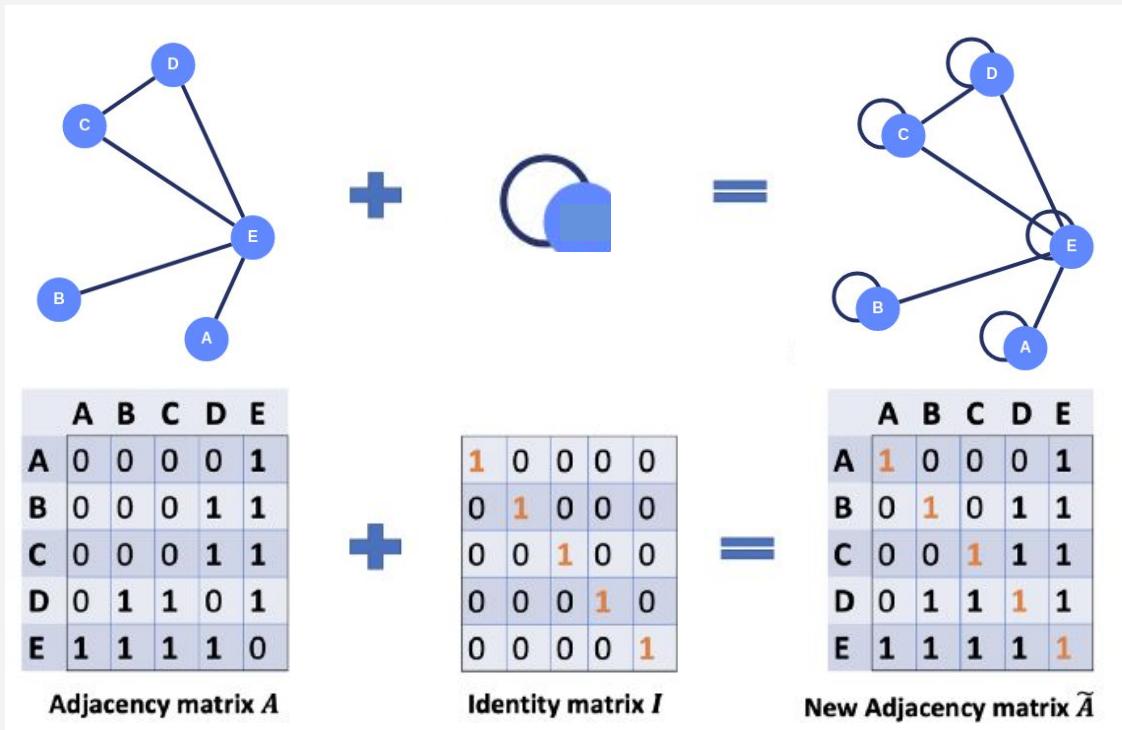
Weighted (undirected)



	A	B	C	D	E	F	G
A	0	8	12	12	12	16	12
B	8	0	0	0	0	0	4
C	12	0	0	0	0	0	0
D	12	0	0	0	0	0	0
E	12	0	0	0	0	0	0
F	16	4	0	0	0	0	12
G	12	0	0	0	0	12	0

# Graphs: Back to basics

**Self-loops:** Incorporating Node Information



# Graphs: Graph Data

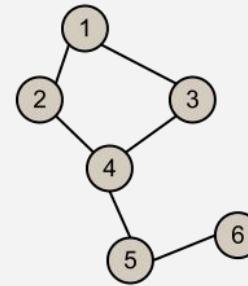
**Edges:** Adjacency Matrix (A)

	1	2	3	4	5	6
1	0	1	1	0	0	0
2	1	0	0	1	0	0
3	1	0	0	1	0	0
4	0	1	1	0	1	0
5	0	0	0	1	0	1
6	0	0	0	0	1	0

```
array([[0, 1, 1, 0, 0, 0],  
       [1, 0, 0, 1, 0, 0],  
       [1, 0, 0, 1, 0, 0],  
       [0, 1, 1, 0, 1, 0],  
       [0, 0, 0, 1, 0, 1],  
       [0, 0, 0, 0, 1, 0]])
```

A: shape(6, 6)

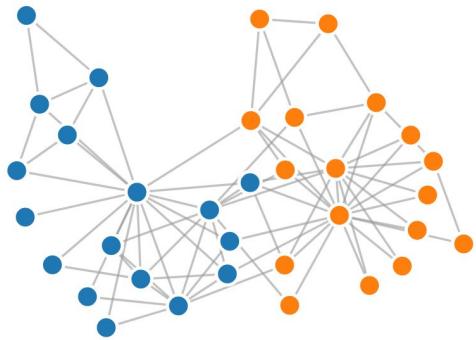
**Nodes:** Node Feature Matrix (X)



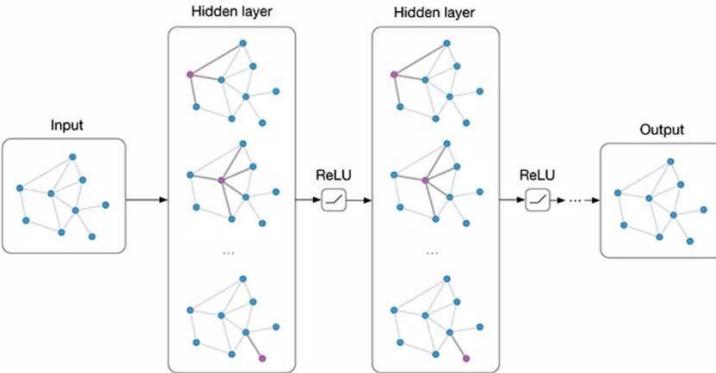
```
array([[ 0.5 , -0.14,  0.65,  1.52],  
       [-0.23, -0.23,  1.58,  0.77],  
       [-0.47,  0.54, -0.46, -0.47],  
       [ 0.24, -1.91, -1.72, -0.56],  
       [-1.01,  0.31, -0.91, -1.41],  
       [ 1.47, -0.23,  0.07, -1.42]])
```

X: shape(6, 4)

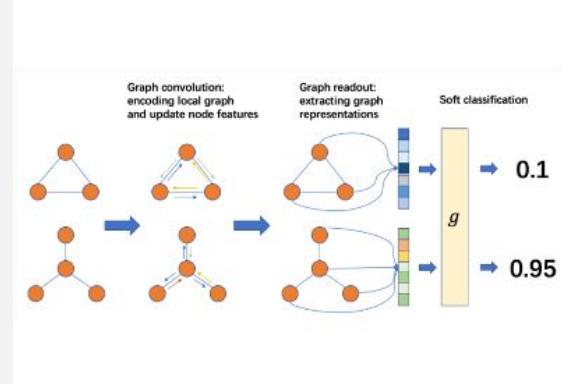
# Graphs: Frameworks & utils



- Store and mutate graphs
- Predefined graph algorithms:
  - Shortest path
  - Dijkstra
  - Clustering
  - Centrality
- Network analysis
- Visualization tools



- An extension library for pyTorch
- Top-rated papers use it for implementation
- Long list of ready-to-use methods and algs:
  - *TransformerConf (2020)*
  - *GCN2Conv (2020)*
  - *DeeperGCN (2020)*
  - ...

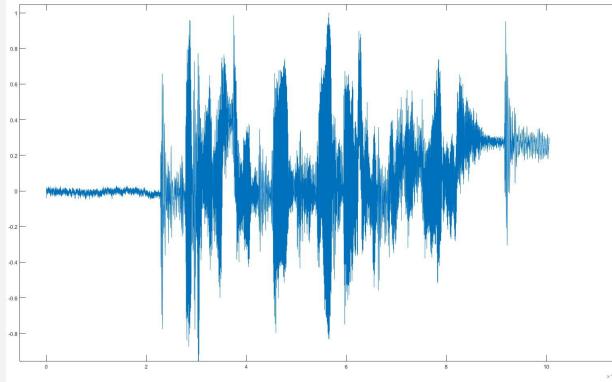


- Building Deep Learning models
- Great tutorials
- Generative graphs
- Very useful for research and advanced tasks
- Supports pyTorch and TensorFlow

### 3. From CNNs to GCNs

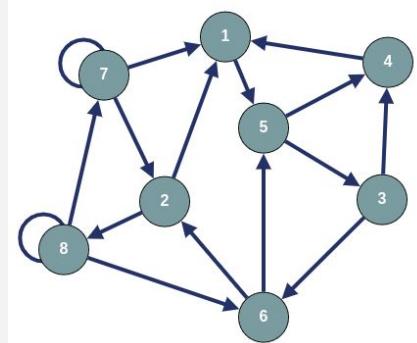
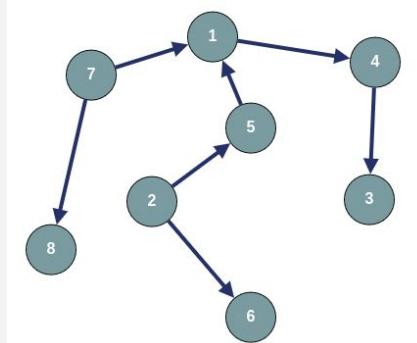
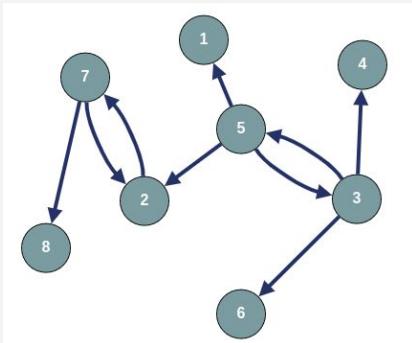
# Image/Sequence vs. Graph Data

Sequential & image data...



Graphs are everywhere !

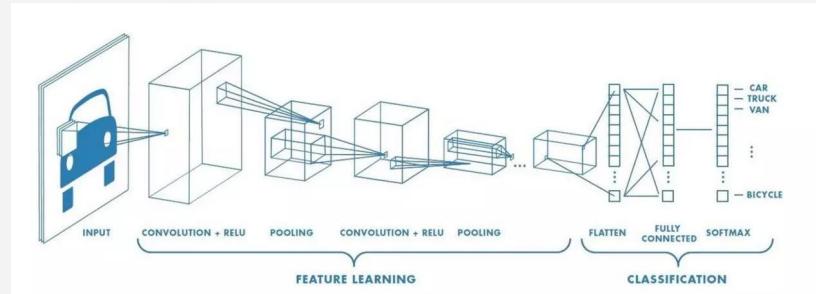
Graph-like data...



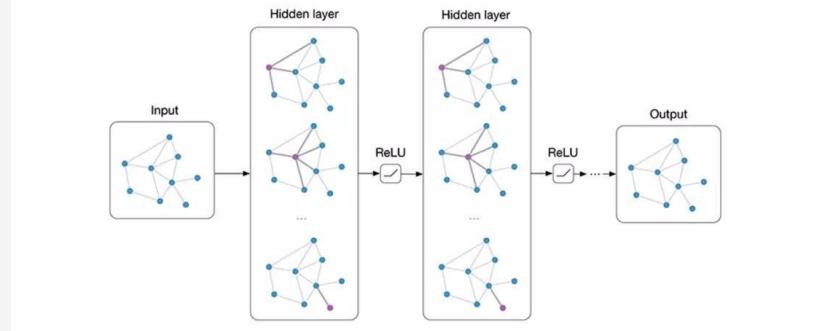
# From CNNs to GCNs

- CNNs leverage the convolutional operator to extract the spatial regularity of the images.
- Graphs can be seen as a strict generalisation of images.
  - Consider any image as a grid graph.
  - Each pixel represents a node
  - Each pixel is adjacent to its 4/8 neighbours
- *Can we adapt the convolutions to operate on graph data ?*

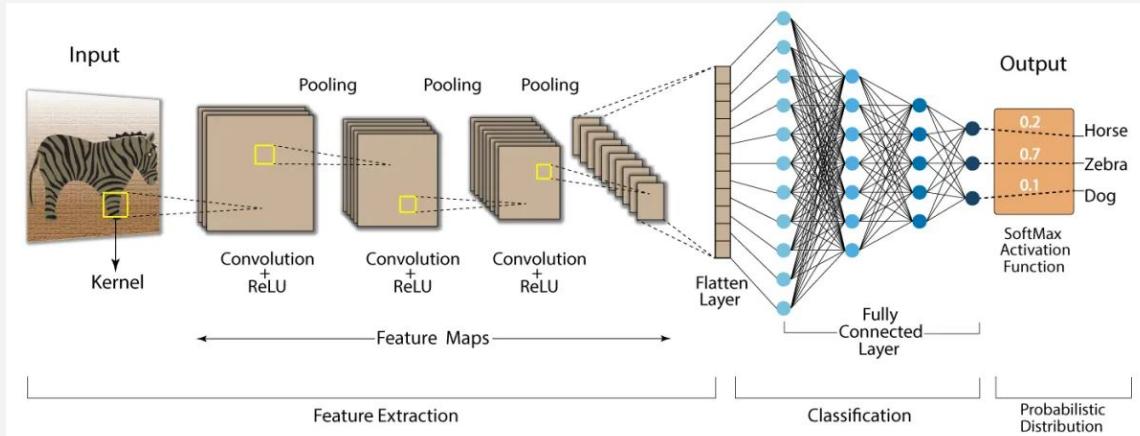
CNNs



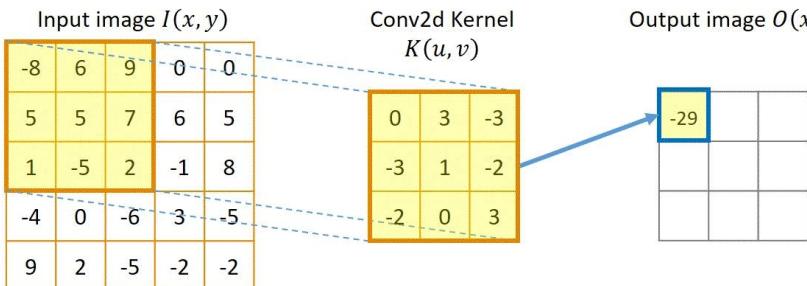
GCNs



# CNN: Convolution on Images



Convolution Neural Network (CNN)



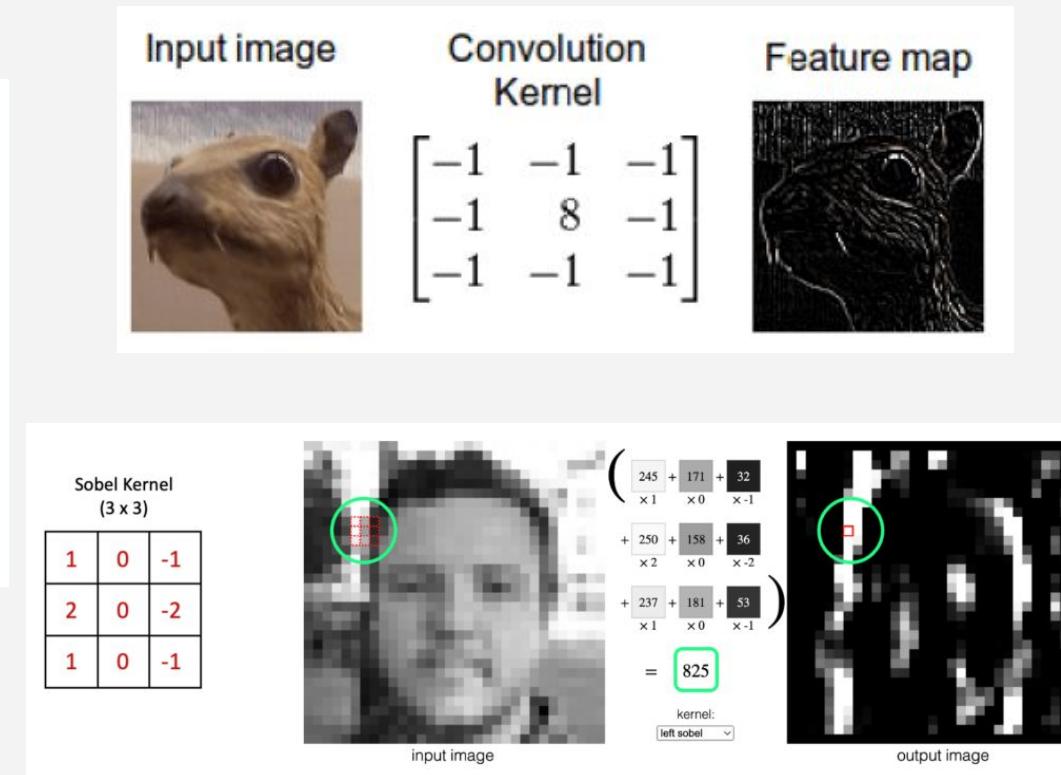
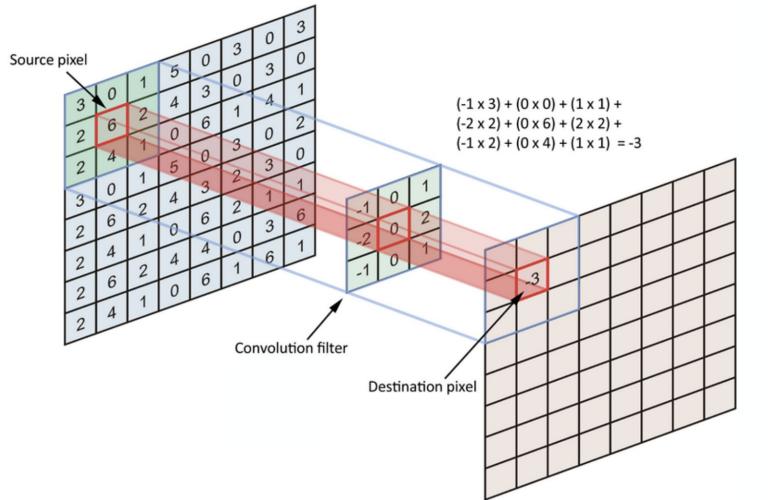
**Update Rule:**

$$H^{(l+1)} = \sigma \left( \sum_{i,j \in \{-1,0,1\}} H_{x+i,y+j}^{(l)} \times W_{i,j}^{(l+1)} \right)$$

shift      input      kernel

# CCN: Convolution on Images

Convolutions capture local patterns and features in images.



# CCN: Convolution on Images

## Convolutions Parameters:

### Parameters

- **in\_channels** (*int*) – Number of channels in the input image
- **out\_channels** (*int*) – Number of channels produced by the convolution
- **kernel\_size** (*int* or *tuple*) – Size of the convolving kernel
- **stride** (*int* or *tuple*, optional) – Stride of the convolution. Default: 1
- **padding** (*int* or *tuple*, optional) – Zero-padding added to both sides of the input. Default: 0
- **padding\_mode** (*string*, optional) – 'zeros', 'reflect', 'replicate' or 'circular'. Default: 'zeros'
- **dilation** (*int* or *tuple*, optional) – Spacing between kernel elements. Default: 1
- **groups** (*int*, optional) – Number of blocked connections from input channels to output channels. Default: 1
- **bias** (*bool*, optional) – If `True`, adds a learnable bias to the output. Default: `True`

### Shape:

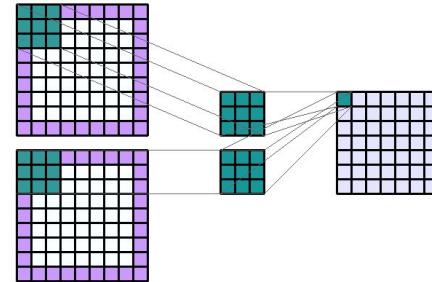
- Input:  $(N, C_{in}, H_{in}, W_{in})$
- Output:  $(N, C_{out}, H_{out}, W_{out})$  where

$$H_{out} = \left\lfloor \frac{H_{in} + 2 \times \text{padding}[0] - \text{dilation}[0] \times (\text{kernel\_size}[0] - 1) - 1}{\text{stride}[0]} + 1 \right\rfloor$$

$$W_{out} = \left\lfloor \frac{W_{in} + 2 \times \text{padding}[1] - \text{dilation}[1] \times (\text{kernel\_size}[1] - 1) - 1}{\text{stride}[1]} + 1 \right\rfloor$$

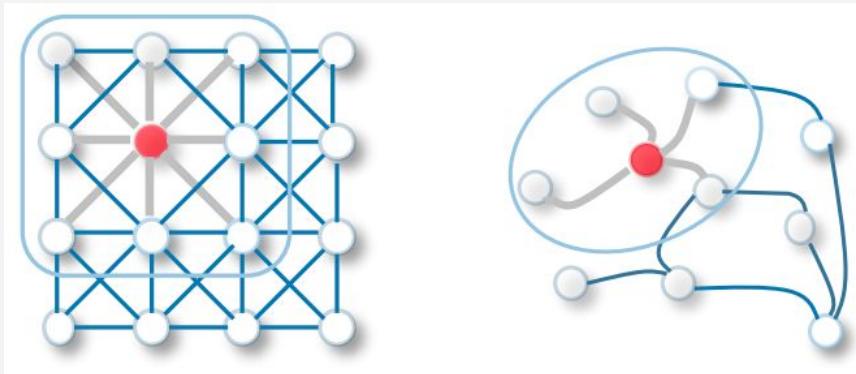
[https://blog.csdn.net/qq\\_34243930](https://blog.csdn.net/qq_34243930)

Stride (*stride = (1, 3)*)  
Padding (*padding = (1, 1)*)



Input: (2, 7, 7) — Output: (1, 7, 7) — K : (3, 3) — P : (1, 1) — S : (1, 1)  
Input shape: (3; r; r) — Output shape: (4; 9; 9) — K : (3, 3) — S : (1, 3)

# Convolution From Image to Graph ?



Convolution on images vs. on graphs

## *On images*

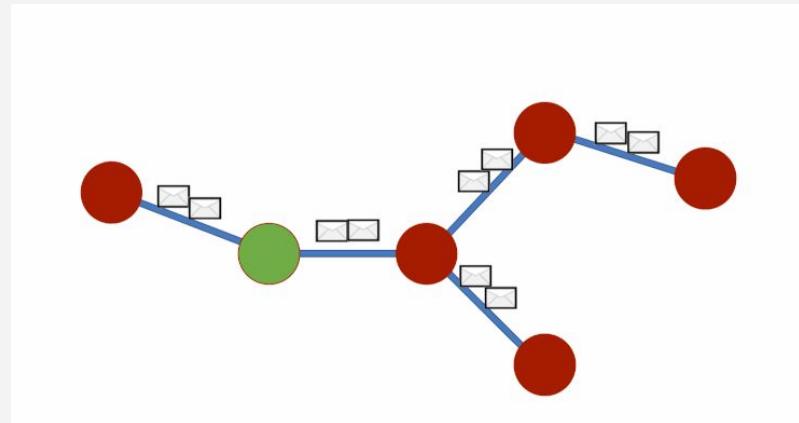
- Convolution works well on Euclidean data, such as image data.
- Convolutions capture local patterns and features in images.
- Convolutions provide a certain level of translation invariance

## *What about graphs?*

- Graphs are non-Euclidean structured data! i.e. they have no “axes”.
- What is a coordinate? And what is a shift?
- Convolutions seem hard to apply to graphs!

## GCN: Convolution on graphs

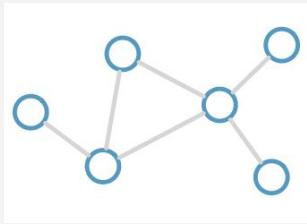
- Convolution can be referred to as Message Passing in GCNs.
- Message passing is performed in the context of a node's local neighborhood.
- Each node shares its current state with its neighbors, and each node's new features are updated accordingly.



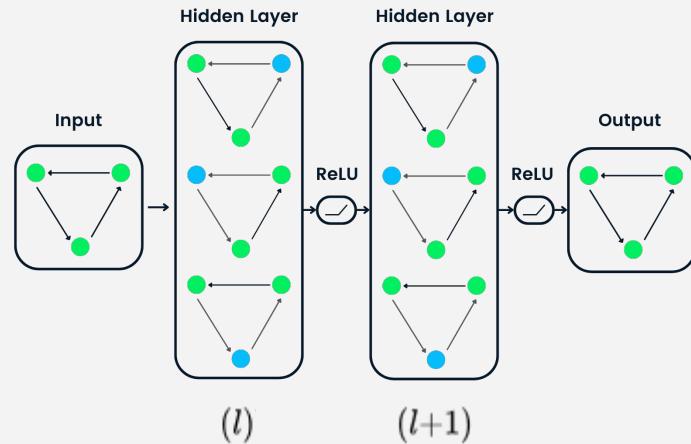
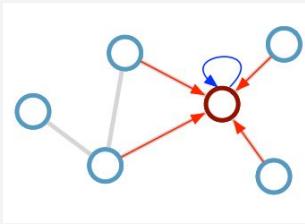
Message Passing

# GCN: Convolution on graphs

Consider this undirected graph:



Calculate update for node in red:



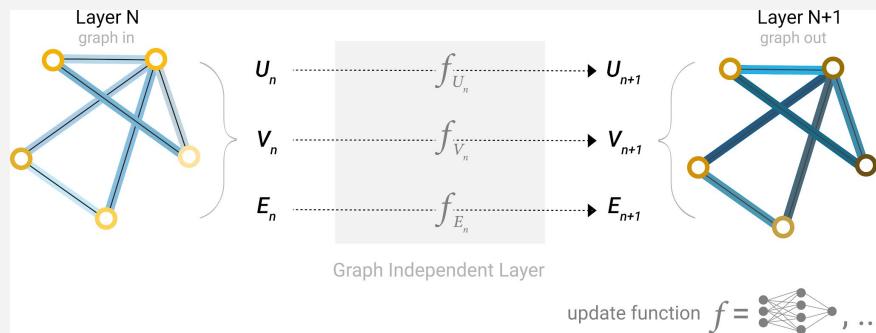
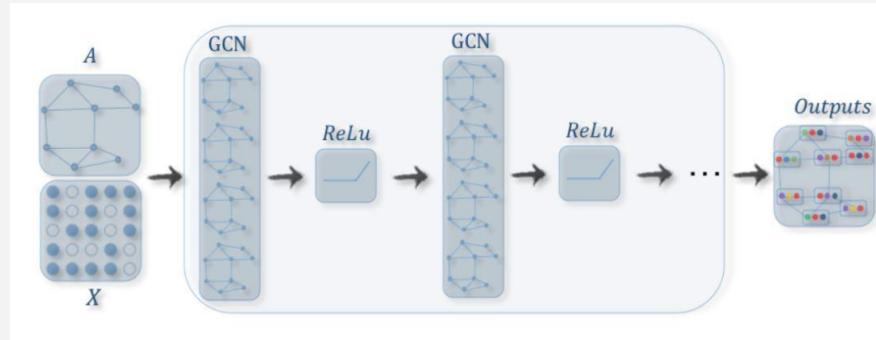
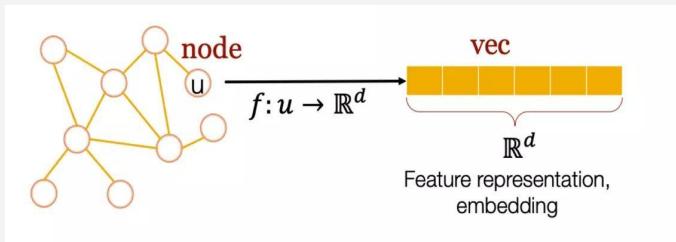
**Update Rule:**

$$H^{(l+1)} = \sigma \left( H_0^{(l)} W^{(l)} + \sum_{j \in \mathcal{N}_i} H_j^{(l)} W^{(l)} + b^{(l)} \right) \quad \text{OR} \quad H^{(l+1)} = \sigma \left( A H^{(l)} W^{(l)} + b^{(l)} \right)$$

# GCN: Convolution on graphs

Why learning embeddings/representations ?

- Projection to a Higher-Dimensional Space
- The higher-dimensional space provides a richer representation that facilitates the learning of complex relationships and patterns in the graph-structured data.
- The final layer's output can be seen as an embedding of nodes in a latent space, where nodes with similar roles or functions in the graph are close together.



# GCN: Convolution on graphs

Let's take a look at an example!

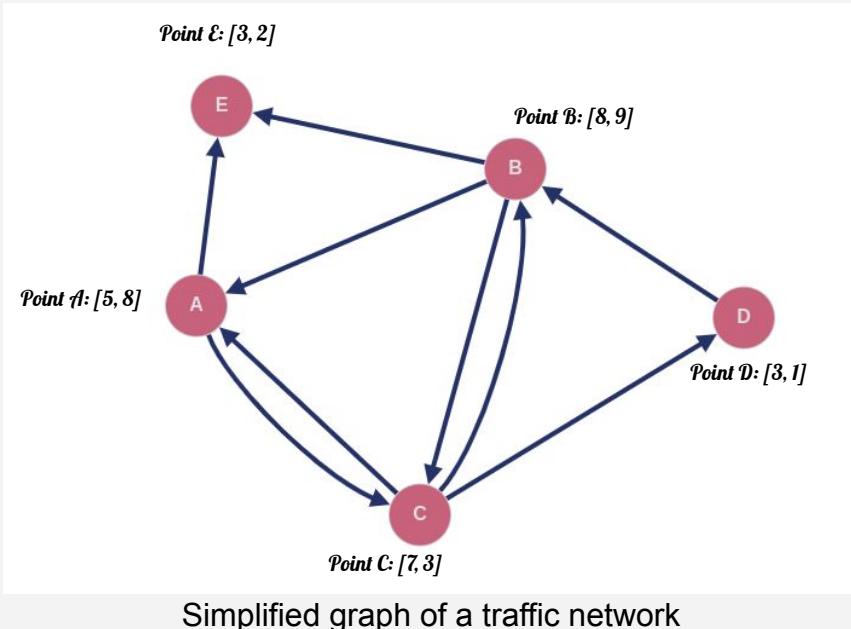
**Do the maths !**

Given the following paper citation graph. Write down the corresponding adjacency matrix  $A$  and the features matrix  $X$ .

$$A = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}; X = \begin{bmatrix} 5 & 8 \\ 8 & 9 \\ 7 & 3 \\ 3 & 1 \\ 3 & 2 \end{bmatrix}; W = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

$$AXW = (A\cancel{X})W$$

$$AX = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 5 & 8 \\ 8 & 9 \\ 7 & 3 \\ 3 & 1 \\ 3 & 2 \end{bmatrix} = \begin{bmatrix} 10 & 5 \\ 15 & 13 \\ 16 & 18 \\ 8 & 9 \\ 0 & 0 \end{bmatrix} \implies AXW = (AX)W =$$



Simplified graph of a traffic network

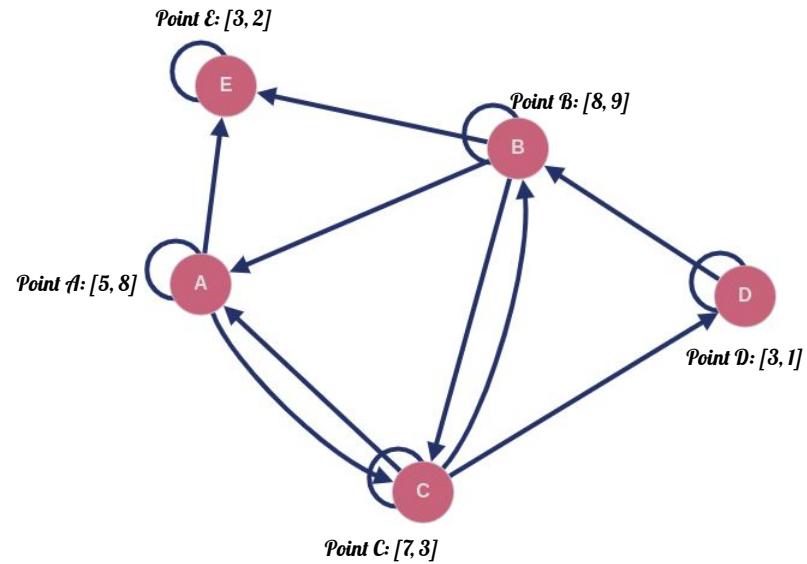
Point X: [road capacity, traffic jam factor]

$$AXW = (AX)W = \begin{bmatrix} 10 & 5 \\ 15 & 13 \\ 16 & 18 \\ 8 & 9 \\ 0 & 0 \end{bmatrix} \times \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 15 & 15 & 15 & 15 \\ 28 & 28 & 28 & 28 \\ 34 & 34 & 34 & 34 \\ 17 & 17 & 17 & 17 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

# GCN: Convolution on graphs

If we add self-loops !

$$A = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}; X = \begin{bmatrix} 5 & 8 \\ 8 & 9 \\ 7 & 3 \\ 3 & 1 \\ 3 & 2 \end{bmatrix}; W = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$



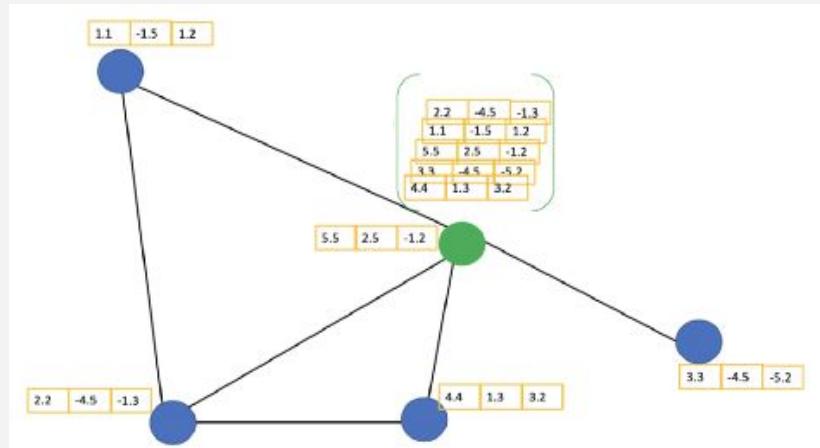
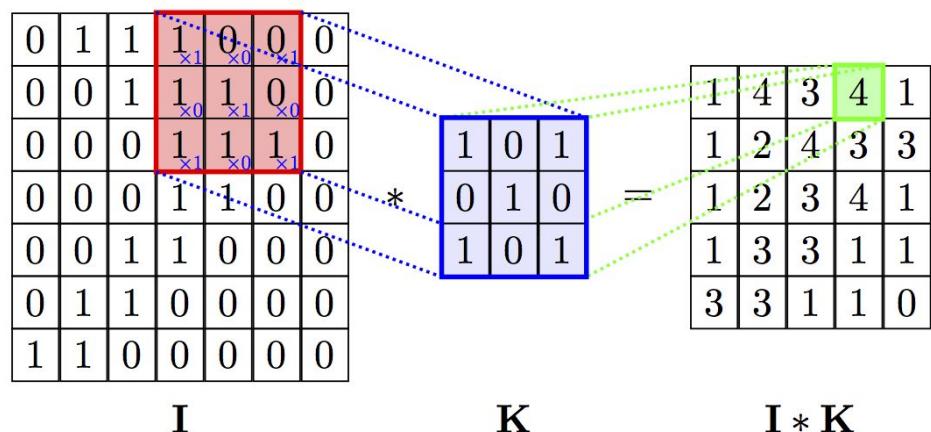
$$AXW = (AX)W$$

Simplified graph of a traffic network

$$AX = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 5 & 8 \\ 8 & 9 \\ 7 & 3 \\ 3 & 1 \\ 3 & 2 \end{bmatrix} = \begin{bmatrix} 15 & 13 \\ 23 & 22 \\ 23 & 21 \\ 11 & 10 \\ 3 & 2 \end{bmatrix} \implies AXW = (AX)W = \begin{bmatrix} 15 & 13 \\ 23 & 22 \\ 23 & 21 \\ 11 & 10 \\ 3 & 2 \end{bmatrix} \times \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 28 & 28 & 28 & 28 \\ 45 & 45 & 45 & 45 \\ 44 & 44 & 44 & 44 \\ 21 & 21 & 21 & 21 \\ 5 & 5 & 5 & 5 \end{bmatrix}$$

## To sum up, convolutional operator for Image vs. Graph

Convolutions on images vs. on graphs

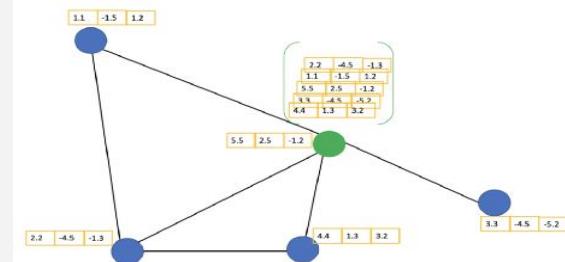
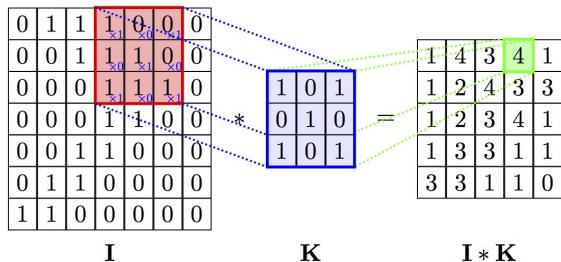


$$H^{(l+1)} = \sigma \left( \sum_{i,j \in \{-1,0,1\}} H_{x+i,y+j}^{(l)} \times W_{i,j}^{(l+1)} \right)$$

$$H^{(l+1)} = \sigma \left( AH^{(l)}W^{(l)} + b^{(l)} \right)$$

# To sum up, convolutional operator for Image vs. Graph

Convolutions on images vs. on graphs



## Local Receptive Fields:

- Convolutional operations are applied using small filters (kernels) that slide over the input image.
- Each filter looks at a local receptive field (a small region of the image).

## Parameter Sharing:

- Parameters (weights) of the filters are shared across the entire image.
- The same set of weights is applied to different local receptive fields.

## Aggregation of Information:

- Aggregate information by computing a weighted sum of the values in the receptive field.

## Local Neighborhoods:

- Message passing occurs over the graph structure where nodes represent entities, and edges represent relationships.
- Message passing is performed in the context of a node's local neighborhood.

## Parameter Sharing:

- GCNs use learnable parameters (weights) associated with edges to determine how information is shared between connected nodes.
- The same set of parameters is shared across all nodes in the graph.

## Aggregation of Information:

- Aggregation is typically performed by computing a weighted sum of neighbor node features.

# GCNs: Convolutional Operator

Graph convolution implementation in *pytorch*:

```
1 import torch.nn as nn
2
3 class GraphConvolution(nn.Module):
4     """
5         Simple GCN layer, similar to https://arxiv.org/abs/1609.02907
6     """
7     def __init__(self, in_features, out_features, bias=True):
8         super(GraphConvolution, self).__init__()
9         self.in_features = in_features
10        self.out_features = out_features
11        self.weight = Parameter(torch.FloatTensor(in_features, out_features))
12        if bias:
13            self.bias = Parameter(torch.FloatTensor(out_features))
14        else:
15            self.bias = None
16        self.activation = nn.ReLU()
17
18    def forward(self, input, adj):
19        support = torch.mm(input, self.weight)
20        output = torch.spmm(adj, support)
21        if self.bias is not None:
22            output = output + self.bias
23        return self.activation(output)
```

$$H^{(l+1)} = \sigma \left( AH^{(l)} W^{(l)} + b^{(l)} \right)$$

$H^{(l)}$   
 $AH^{(l)}$   
 $W^{(l)}$   
 $b^{(l)}$

**Shapes:**

$$A \in \mathbb{R}^{n \times n}$$

$$H^{(l)} \in \mathbb{R}^{n \times d}$$

$$W^{(l)} \in \mathbb{R}^{d \times d'}$$

$$b^{(l)} \in \mathbb{R}^{d'}$$

- $n$ : number of nodes
- $d$ : `in_features`
- $d'$ : `out_features`

⇒

$$AH^{(l)} \in \mathbb{R}^{n \times d}$$

$$AH^{(l)} W^{(l)} \in \mathbb{R}^{n \times d'}$$

$$AH^{(l)} W^{(l)} + b^{(l)} \in \mathbb{R}^{n \times d'}$$

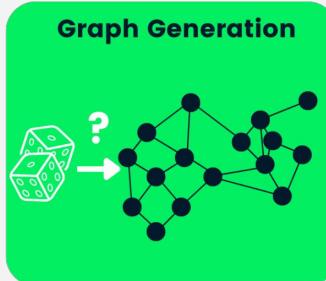
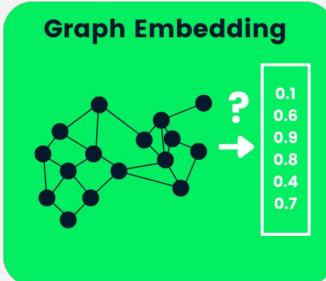
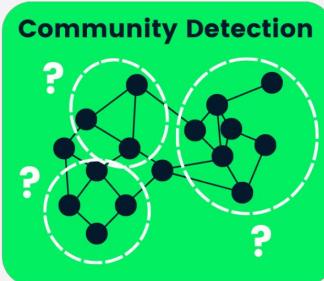
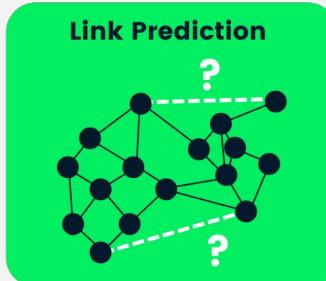
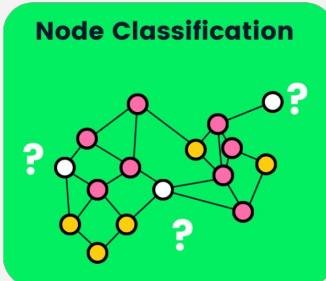
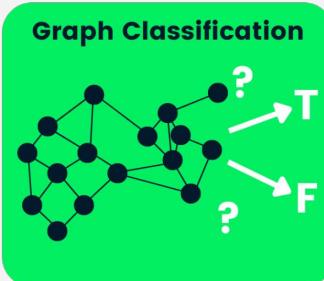
**Mathematically:**

$$f : \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$$

$$X \mapsto AXW + b$$

## 4. GCNs: Practical Aspects

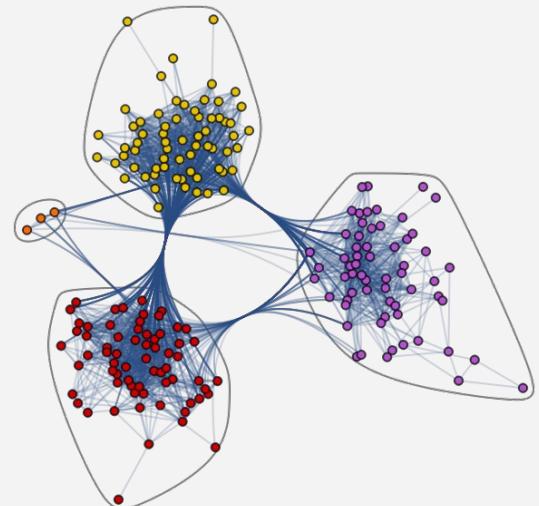
# Tasks on Graphs



## Tasks on Graphs: Node classification

- **Node classification:** Predict a type of a given node

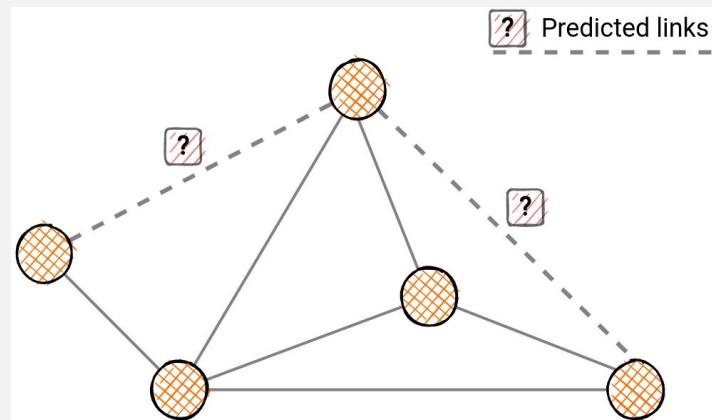
e.g., Malicious users in a social network, community clustering, etc



## Tasks on Graphs: Link prediction

- **Link prediction:** Predict whether two nodes are linked

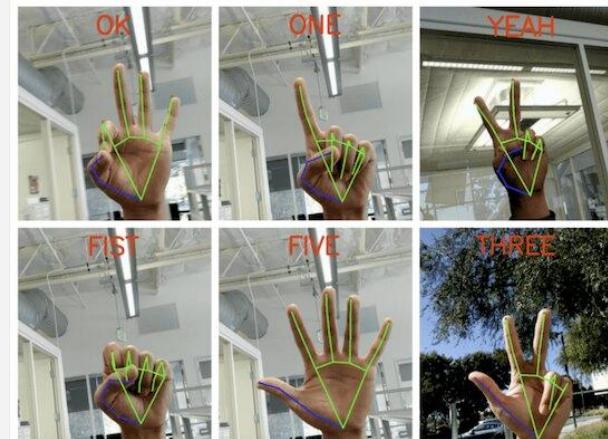
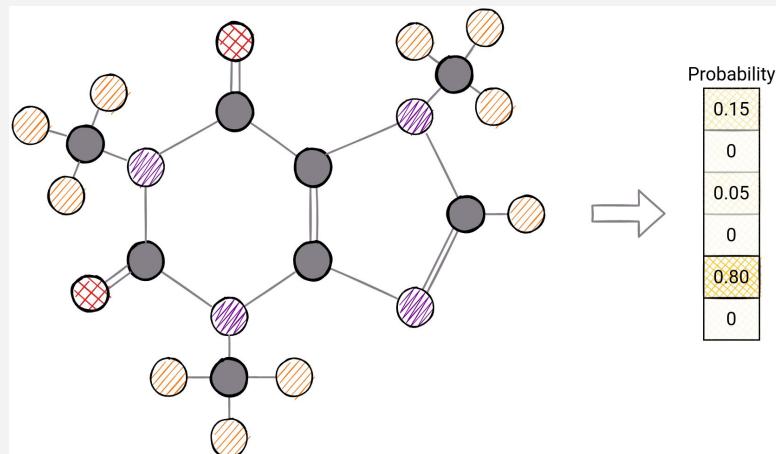
e.g., protein-protein interaction, friend suggestion, etc



## Tasks on Graphs: Graph classification

- **Graph classification:** Predict the class of a given graph

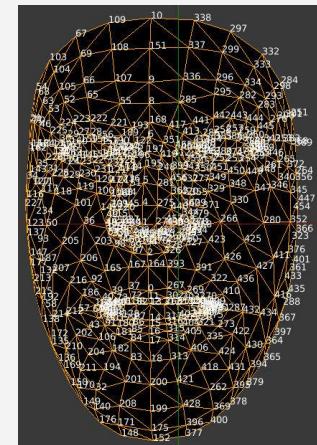
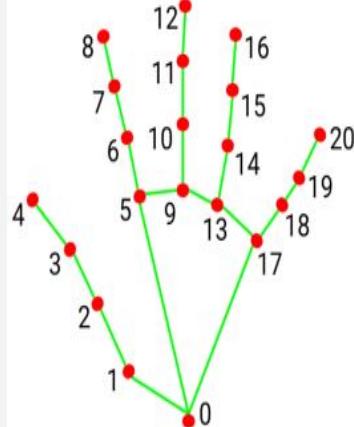
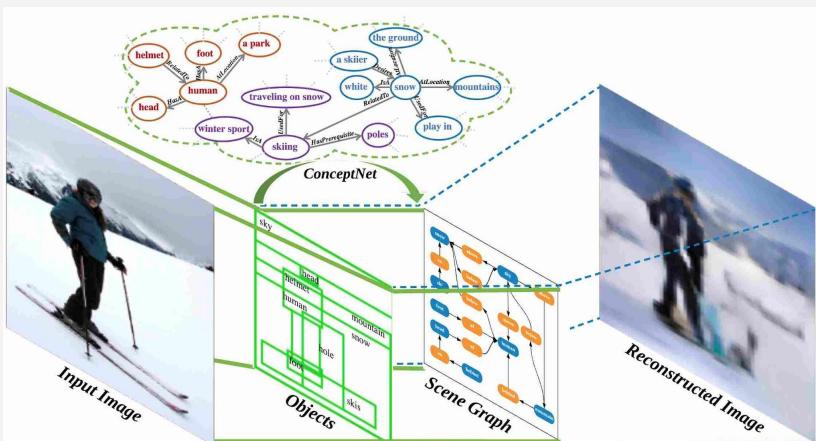
e.g., type of a chemical molecule, gesture recognition, etc.



# Tasks on Graphs: Graph Generation

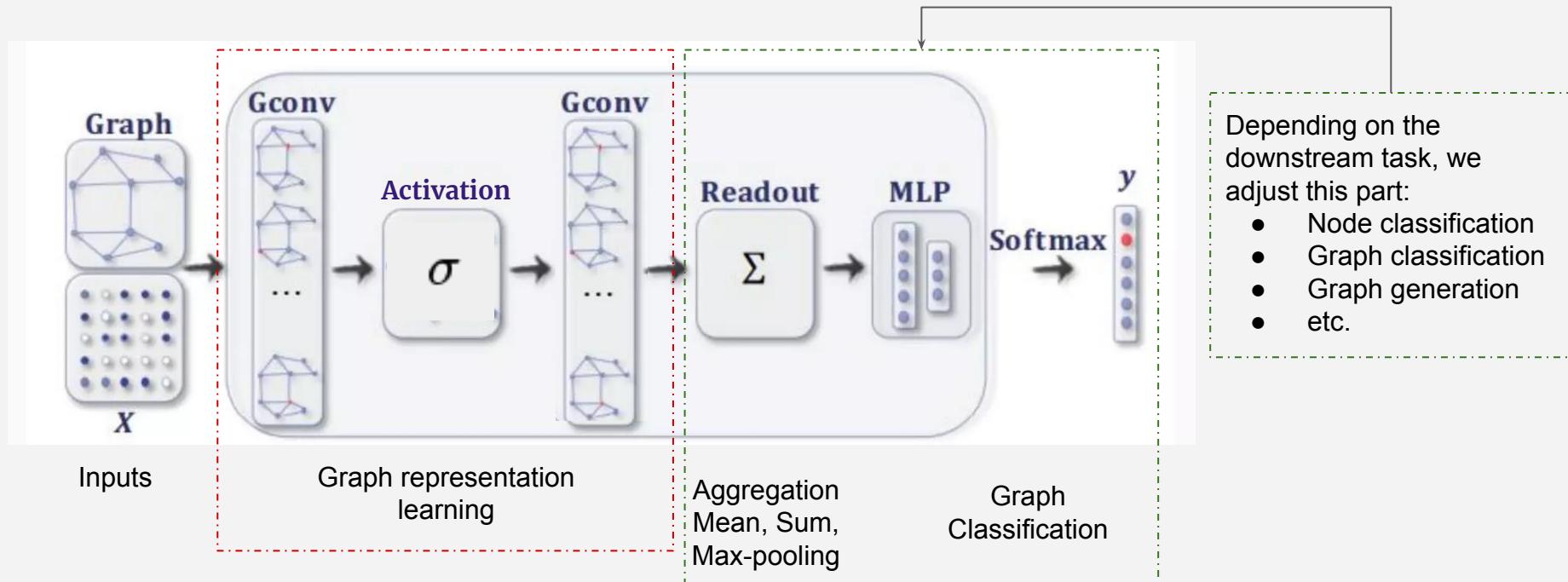
→ **Graph generation:** generate a graph given an input data.

e.g., interactions learning, molecule generation, interactions sparsifying, etc.



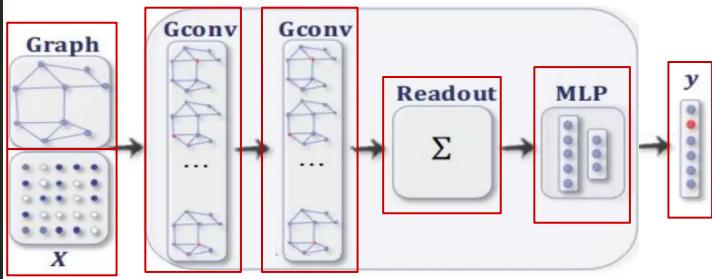
- |                       |                       |
|-----------------------|-----------------------|
| 0. WRIST              | 11. MIDDLE_FINGER_DIP |
| 1. THUMB_CMC          | 12. MIDDLE_FINGER_TIP |
| 2. THUMB_MCP          | 13. RING_FINGER_MCP   |
| 3. THUMB_IP           | 14. RING_FINGER_PIP   |
| 4. THUMB_TIP          | 15. RING_FINGER_DIP   |
| 5. INDEX_FINGER_MCP   | 16. RING_FINGER_TIP   |
| 6. INDEX_FINGER_PIP   | 17. PINKY_MCP         |
| 7. INDEX_FINGER_DIP   | 18. PINKY_PIP         |
| 8. INDEX_FINGER_TIP   | 19. PINKY_DIP         |
| 9. MIDDLE_FINGER_MCP  | 20. PINKY_TIP         |
| 10. MIDDLE_FINGER_PIP |                       |

# Overall Structure of GCN



# Basic GCN Implementation

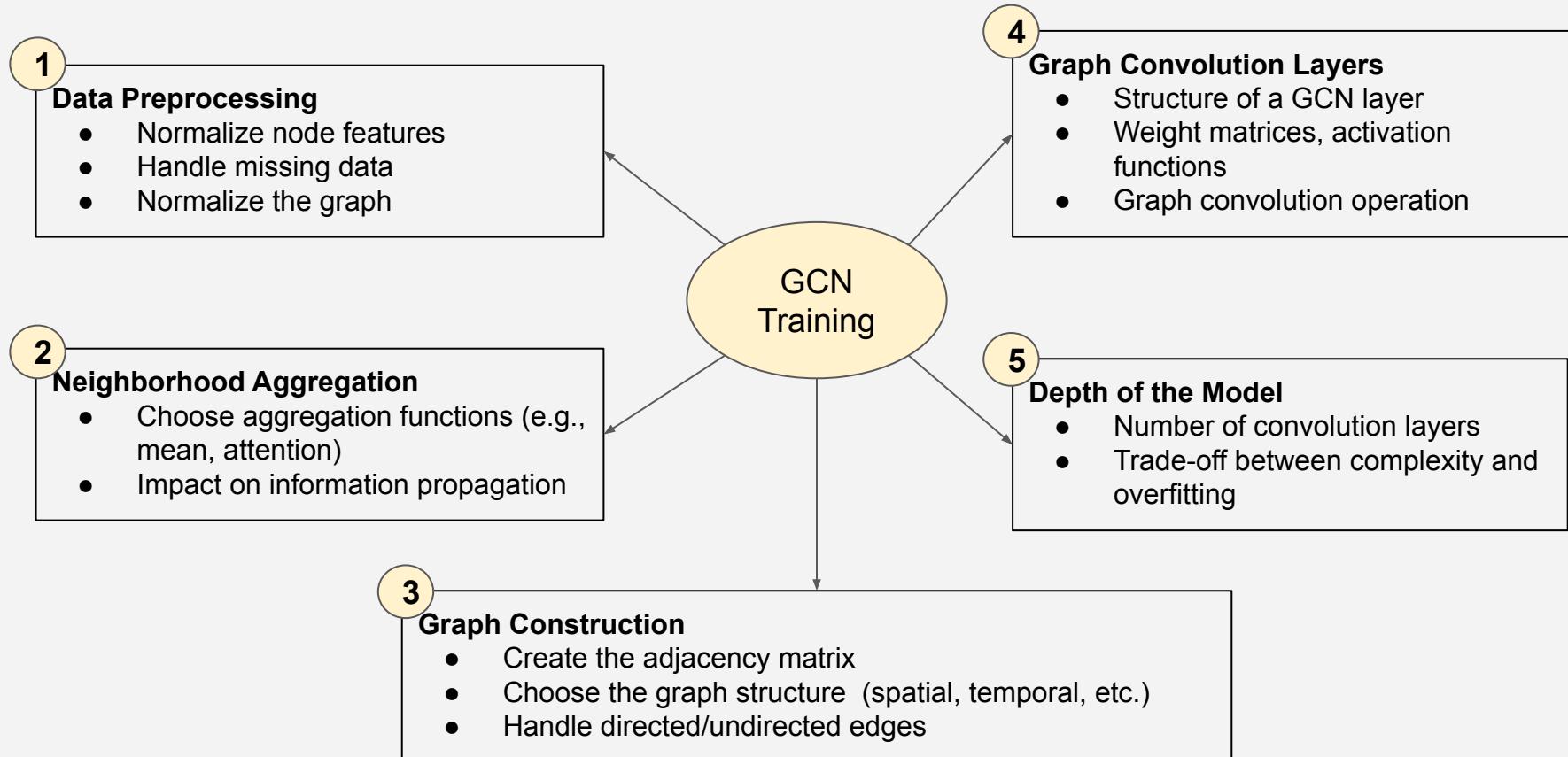
```
1 class GCN(nn.Module):
2     def __init__(self, in_dim, n_nodes, hidden_dim, n_gcn_layers, n_classes, dropout):
3         super(GCN, self).__init__()
4         ## GCN layers to learn graph representation
5         self.gc1 = GraphConvolution(in_dim, hidden_dim)
6         self.gc2 = GraphConvolution(hidden_dim, hidden_dim)
7
8         ## MLP head to classify the graphs
9         self.mlp = nn.Sequential(
10             nn.Linear(hidden_dim * n_nodes, 64),
11             nn.ReLU(),
12             nn.Linear(64, n_classes)
13         )
14
15         ## dropout parameter to prevent overfitting
16         self.dropout = dropout
17
18     def forward(self, x, adj):
19
20         ## first gcn layer with activation function and dropout
21         x = F.relu(self.gc1(x, adj))
22         x = F.dropout(x, self.dropout, training=self.training)
23
24         ## second gcn layer with activation function and dropout
25         x = F.relu(self.gc2(x, adj))
26         x = F.dropout(x, self.dropout, training=self.training)
27
28         ## reshape x from (b, n_joints, hidden_dim) into (b, n_joints * hidden_dim)
29         b, _, _ = x.shape
30         x = x.view(b, -1)
31
32         ## mlp for classification
33         out = self.mlp(x)
34
35         return out
```



## Parameters:

- $in\_dim$ : number of features of  $X$
- $n\_nodes$ : number of nodes in the graph.
- $hidden\_dim$ : embedding dimension
- $n\_gcn\_layers$ : number of convolutional layers
- $n\_classes$ : number of classes

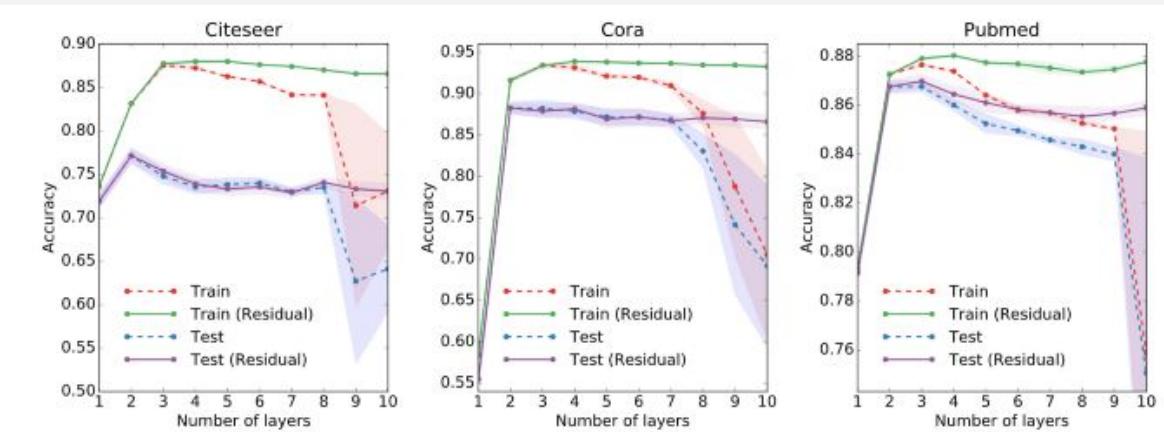
# Training GCNs: Key considerations



## Practical advices

Potential Pitfalls when going deep:

- Vanishing gradient
- Overfitting
- Over-smoothing: node vectors become too similar
- Bottleneck(over-squashing): a single node vector contains data of too many nodes



Model	2-Layer	4-Layer	8-Layer	16-Layer	32-Layer	64-Layer
GCN-res	$88.18 \pm 1.59$	$86.50 \pm 1.87$	$84.83 \pm 1.93$	$78.60 \pm 4.28$	$59.82 \pm 7.74$	$39.71 \pm 5.15$
PairNorm	$79.98 \pm 3.80$	$82.32 \pm 2.79$	$81.52 \pm 3.66$	$82.29 \pm 2.62$	$81.91 \pm 2.45$	$81.72 \pm 2.82$
NodeNorm	$89.53 \pm 1.29$	$88.60 \pm 1.36$	$88.02 \pm 1.67$	$88.41 \pm 1.25$	$88.30 \pm 1.30$	$87.40 \pm 2.06$

<https://arxiv.org/abs/2006.07107> - Effective Training Strategies for Deep Graph Neural Networks

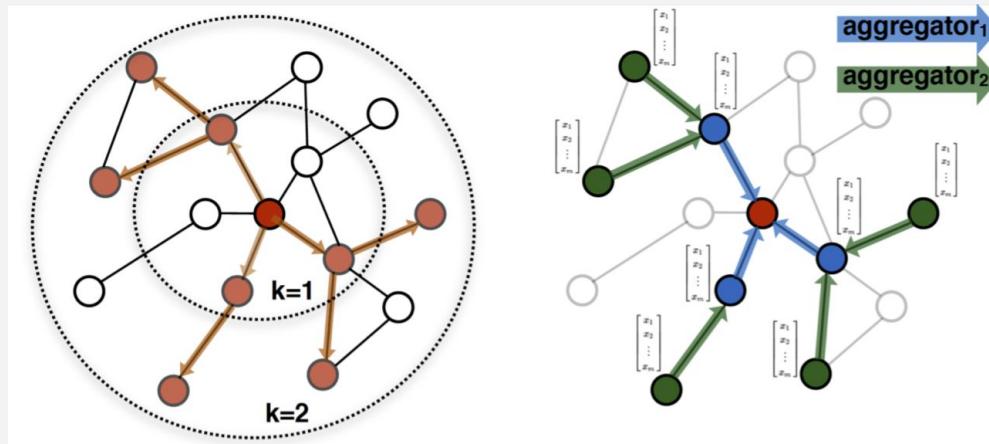
## More advanced GCNs variantes

### → GraphSAGE (Graph Sample and Aggregated)

"Inductive Representation Learning on Large Graphs" by Hamilton et al. (2017).

#### Key Idea:

GraphSAGE addresses scalability issues by sampling a fixed-size neighborhood around each node during training. It aggregates information from the sampled neighbors, allowing it to scale to large graphs.



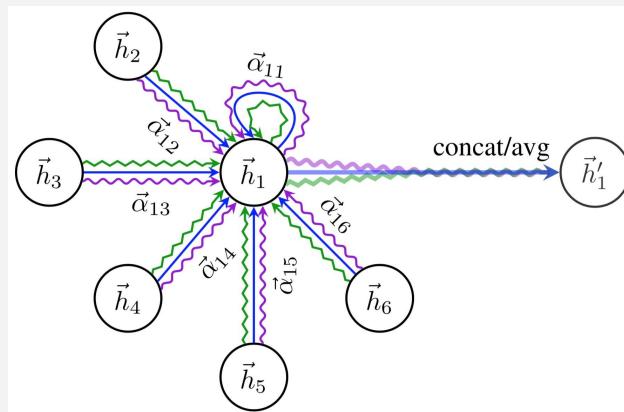
## More advanced GCNs variantes

### → GAT (Graph Attention Network)

"Graph Attention Networks" by Velickovic et al. (2018).

#### Key Idea:

GAT introduces attention mechanisms to assign different weights to neighbors during aggregation, enabling nodes to selectively attend to more informative neighbors.



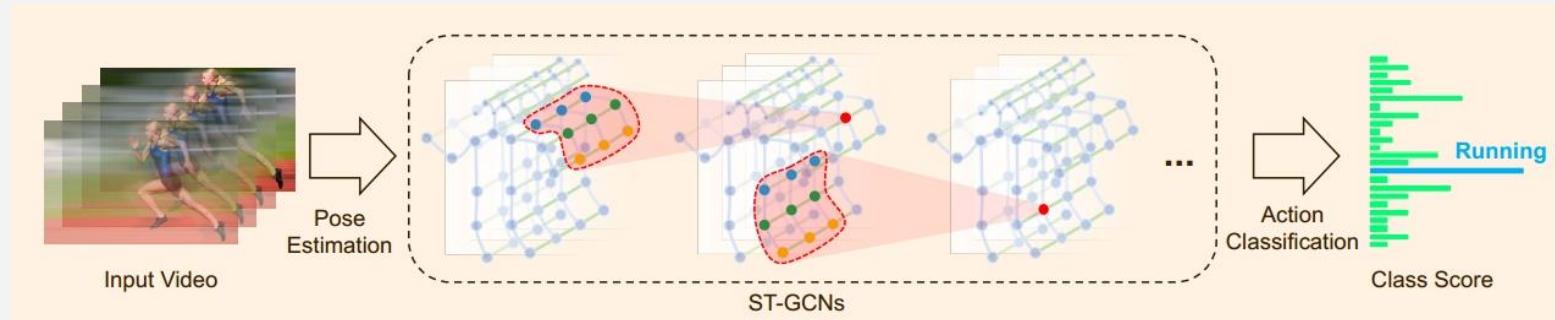
## More advanced GCNs variantes

### → STGCN (Spatial Temporal Graph Convolutional Networks)

“Spatial Temporal Graph Convolutional Networks for Skeleton-Based Action Recognition” by Yan et al. (2018).

#### Key idea:

STGCN incorporates both spatial and temporal dependencies within a graph structure. It applies graph convolutions across both spatial and temporal dimensions. This enables the model to capture spatial dependencies between different locations as well as temporal dependencies over time.



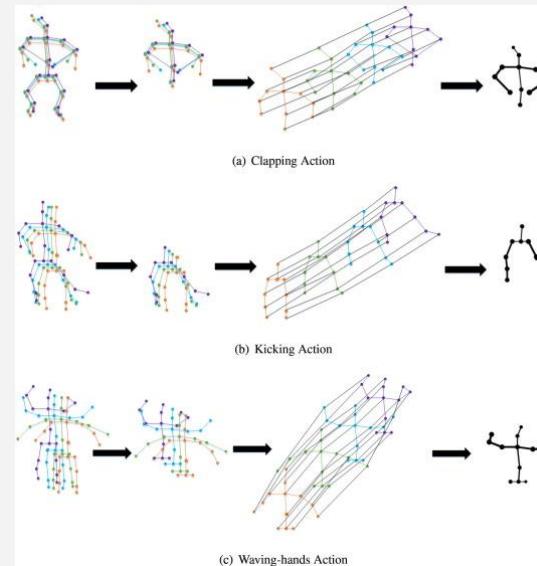
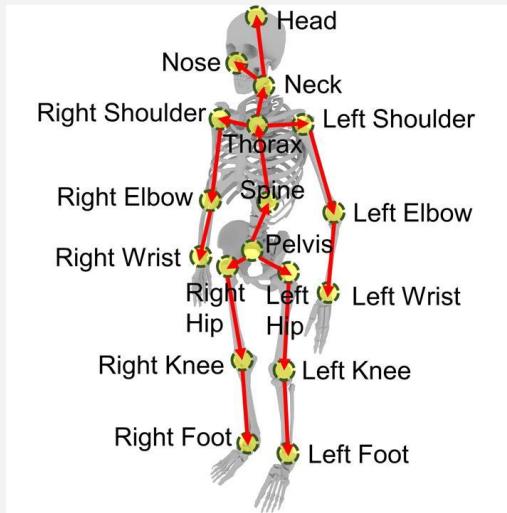
## More advanced GCNs variantes

### → SGCN (Sparse Graph Convolution Network)

“Sparse graph convolution network for pedestrian trajectory prediction” by Shi et al. (2021)

#### Key idea:

SGCNs are designed to be efficient for graphs with a sparse adjacency matrix. One of the main motivations for SGCNs is to reduce the computational complexity associated with standard GCNs, which involve matrix multiplications with the full adjacency matrix.



# Challenges & Future Directions: What lies ahead

## → Scalability

Challenge: As the size of the graph increases, the computational and memory requirements for training and inference increases.

Future Direction: Developing scalable GCN variants or exploring techniques to efficiently handle large-scale graphs.

## → Handling Noisy or Incomplete Graphs

Challenge: Graphs in real-world applications often contain noise, missing edges, or incomplete information.

Future Direction: Developing GCN variants that are robust to noisy data or designing methods to impute missing information in graphs.

## → Generalization to Heterogeneous Data

Challenge: Generalizing GCNs to handle heterogeneous graphs with different types of nodes and edges is a challenge.

Future Direction: the development of more flexible and adaptive architectures to handle heterogeneous graphs.

## → Interpretable Graph Representations

Challenge: Understanding and interpreting the learned representations in GCNs can be challenging, especially in complex, high-dimensional graphs.

Future Direction: Exploring techniques for interpretability and visualization of graph representations.

## Take home notes

- GCNs are used for learning on the graph.
- GCNs use both node features and the structure for the training
- The main idea of the GCN is to take the weighted average of all neighbors' node features (including itself): Lower-degree nodes get larger weights. Then, we pass the resulting feature vectors through a neural network for training.
- We can stack more layers to make GCNs deeper. Normally, we go for 2 or 3-layer GCN.



## Additional Resources

- <https://github.com/Jiakui/awesome-gcn>
- <https://antonsruberts.github.io/graph/gcn/>
- <https://ieeexplore.ieee.org/ielaam/5962385/9312808/9046288-aam.pdf>
- <https://distill.pub/2021/gnn-intro/>
- <https://distill.pub/2021/understanding-gnns/>

## Practical Example: GCN Training for Static Hand Gesture Recognition

